1,1,2,2-Tetrahydroperfluoro-1-decanol 678-39-7 | DTXSID7029904

Model Performance

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Model	II)ata
IVIOGCI	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: 4.29

Global applicability domain: Inside

Local applicability domain index: 9.48e-01

Confidence level: 5.88e-01

Nearest Neighbors from the Training Set

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Dipropylamine Measured: 3.59 Predicted: 4.37 Image not found

Piperidine Measured: 4.04 Predicted: 4.32 Image not found

1-Pentanol Measured: 4.69 Predicted: 4.17

Image not found

1-Hexanol Measured: 5.18 Predicted: 4.67 Image not found

Isopentyl alcohol Measured: 4.52 Predicted: 4.24